Perfluorotributylamine

	•	omaorombatylamino	
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Model Performance

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N	Model	Data	

Weighted KNN model

5-fold CV	(75%)	Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.95	0.69	0.95	0.65	0.96	0.68	

Model Results

Predicted value: 2.43

Global applicability domain: Inside

Local applicability domain index: 9.92e-01

Confidence level: 7.37e-01

Nearest Neighbors from the Training Set

Image not found

Propanal

Measured: 3.02 Predicted: 2.43 Image not found

Measured: 2.31

Acetone

Predicted: 2.42

Image not found

Ethyl formate
Measured: 2.19
Predicted: 2.41

Image not found

Methyl acetate
Measured: 2.31
Predicted: 2.41

Image not found

Dichloromethane Measured: 2.27 Predicted: 2.41